

Magnetic Response of Interacting Electrons in a Fractal Network: A Mean Field Approach

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The Hubbard model on a Sierpinski gasket fractal is carefully examined within a Hartree-Fock mean field approach. We examine the influence of a magnetic flux threading the gasket on its ground state energy, persistent current and the Drude weight. Both an isotropic gasket and its anisotropic counterpart have been examined. The variance in the patterns of the calculated physical quantities are discussed for two situations, viz, at half-filling and when the ‘band’ is less than half-filled. The phase reversal of the persistent currents and the change of the Drude weight as a function of the Hubbard interaction are found to exhibit interesting patterns that have so far remained unaddressed.

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I. INTRODUCTION

Deterministic fractals have been known to bridge the gap between systems possessing perfect periodic order and the completely random ones. The spectrum of non interacting electrons on such lattices has been exhaustively investigated in the past [1–23]. The principal characteristic features of a deterministic fractal may be summarized as follows: First, the energy spectrum is a Cantor set, and its degenerate [1]. Second, the density of states displays a variety of singularities and a magnetic field is shown to broaden up the spectrum [3, 4], and third, the electronic conductance exhibits scaling with a multi-fractal distribution of the exponents [11]. Apart from these, in certain cases, isolated extended eigenstates also appear in deterministic, finitely ramified fractal lattices [24–27], and extensive numerical work has recently proposed a possible existence of even a continuum of such extended states [28].

However, the typical properties exhibited by the deterministic fractals are obtained within the picture of non-interacting spinless Fermions. The very fundamental questions such as whether the spectral peculiarities exist even in the presence of say, electron-electron interaction, or whether the response of a fractal lattice to an externally applied magnetic (or electric) field brings out any new features when one looks beyond the non-interacting picture, are still to be addressed. The effect of electron-electron interaction on the spectral properties are, to our mind, is of great importance, particularly because of several experiments done on fractal networks that studied the magnetoresistance, the superconductor-normal phase boundaries on Sierpinski gasket wire networks [6–8, 21, 22]. These experiments, together with the earlier ones on regular square or honeycomb networks [29, 30] to study the flux quantization effects pioneered the actual observational studies of spectral properties of planar networks and the Aharonov-Bohm effect in systems with or without translational invariance. Although in an early paper the problem of interacting electrons on a percolating cluster that displays a fractal geometry [31], has

been addressed, to the best of our knowledge, no rigorous effort has been made so far to unravel the effect of an interplay of electron-electron interaction and an external magnetic field on deterministic networks such as a Sierpinski gasket (SPG), even at a mean field level.

This inspires us to undertake a detailed study of the ground state energy and the magnetic response of a Sierpinski gasket (SPG) fractal [1–3] that stands out to be a classic example of such lattices, and has been the subject of the experiments cited above. We examine the persistent current [32, 33] in such a fractal in the presence of on-site Hubbard interaction within an unrestricted Hartree-Fock mean field scheme. Persistent current in normal metal loops [32–35] is an important effect in mesoscopic dimensions. Here, an SPG network offers a unique opportunity to study the persistent current in a self-similar distribution of loops, and with correlated electrons it is likely to give rise to new observations. This is a major motivation of the present work.

Apart from this, the magnetoconductance (Drude weight) has also been calculated and the variation of the response of the lattice to the external magnetic field has been carefully studied as the fractal grows in size. To the best of our knowledge the interplay of a fractal geometry and electron-electron correlation in the form of persistent currents and the Drude weight has not been studied before. With the metallic SPG networks already synthesized, the present study may motivate experiments for a direct observation of the effects presented here. In particular, based on the success of the lithographic techniques it may not be too wild an idea to suggest an SPG kind of fractal network built by carbon nanotubes that are connected at the vertices.

As mentioned before, we examine both the isotropic and the anisotropic SPG fractal networks. The anisotropy is introduced only in the values of the nearest-neighbor hopping integrals. The response of the lattice is found to differ grossly for an anisotropic system compared to the isotropic one. This is of course, dependent on the relative values of the parameters in the Hamiltonian, through which the anisotropy enters the system.

For example, the anisotropic SPG fractal is found to be more conducting than the isotropic one in the sense that, the lattice remains conducting over a wide range of values of the Hubbard interaction. The magnitude of the conductivity however, is sensitive to the strength of the hopping parameters. This fact has also been reported recently for non-interacting electrons [36].

In what follows, we present the results. In section II, the model Hamiltonian is presented. Section III briefly describes the mean field approach, while the results and the discussion are included in section IV. In section V we draw our conclusions.

II. THE MODEL

We start by referring to Fig. 1 where a 3-rd generation SPG in which each elementary plaquette is threaded by a magnetic flux ϕ (measured in unit of the elementary flux quantum $\phi_0 = ch/e$) is shown. The filled black circles

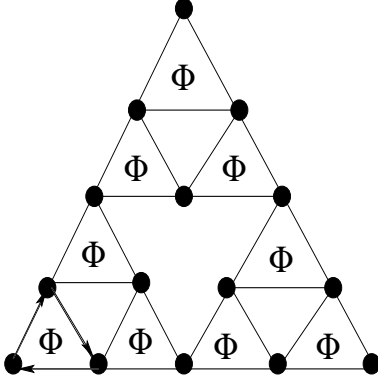


FIG. 1: A 3-rd generation Sierpinski gasket in which each elementary plaquette is penetrated by a magnetic flux ϕ . The filled black circles correspond to the positions of the atomic sites.

cles correspond to the positions of the atomic sites in the SPG. To describe the system we use a tight-binding framework. In a Wannier basis the Hamiltonian reads,

$$H_{\text{SPG}} = \sum_{i,\sigma} \epsilon_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \sum_{\langle ij \rangle, \sigma} t \left[e^{i\theta} c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right] + \sum_i U c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \quad (1)$$

where, $\epsilon_{i\sigma}$ is the on-site energy of an electron at the site i of spin σ (\uparrow, \downarrow) and t is the nearest-neighbor hopping strength. In the case of an anisotropic SPG, the anisotropy is introduced only in the nearest-neighbor hopping integral t which takes on values t_x and t_y for hopping along the *horizontal* and the *angular* bonds, respectively. Due to the presence of magnetic flux ϕ , a phase factor $\theta = 2\pi\phi/3$ appears in the Hamiltonian when an electron hops from one site to another site, and accordingly, a negative sign comes when the electron hops

in the reverse direction. As the magnetic field associated with the flux ϕ does not penetrate any part of the circumference of the elementary triangle, we ignore the Zeeman term in the above tight-binding Hamiltonian (Eq. 1). $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators, respectively, of an electron at the site i with spin σ . U is the strength of on-site Coulomb interaction.

III. THE MEAN FIELD APPROACH

A. Decoupling of the interacting Hamiltonian

To determine the energy eigenvalues of the interacting model of the SPG described by the tight-binding Hamiltonian given in Eq. 1, first we decouple the interacting Hamiltonian using the generalized Hartree-Fock approach [37, 38]. The full Hamiltonian is completely decoupled into two parts. One is associated with the up-spin electrons, while the other is with the down-spin electrons. The on-site potentials get modified appropriately, and are given by,

$$\epsilon'_{i\uparrow} = \epsilon_{i\uparrow} + U \langle n_{i\downarrow} \rangle \quad (2)$$

$$\epsilon'_{i\downarrow} = \epsilon_{i\downarrow} + U \langle n_{i\uparrow} \rangle \quad (3)$$

where, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator. With these site energies, the full Hamiltonian (Eq. 1) can be written in the decoupled form (in the mean field approximation) as,

$$\begin{aligned} H_{\text{mean field}} &= \sum_i \epsilon'_{i\uparrow} n_{i\uparrow} + \sum_{\langle ij \rangle} t \left[e^{i\theta} c_{i\uparrow}^\dagger c_{j\uparrow} + e^{-i\theta} c_{j\uparrow}^\dagger c_{i\uparrow} \right] \\ &+ \sum_i \epsilon'_{i\downarrow} n_{i\downarrow} + \sum_{\langle ij \rangle} t \left[e^{i\theta} c_{i\downarrow}^\dagger c_{j\downarrow} + e^{-i\theta} c_{j\downarrow}^\dagger c_{i\downarrow} \right] \\ &- \sum_i U \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \\ &= H_\uparrow + H_\downarrow - \sum_i U \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \end{aligned} \quad (4)$$

where, H_\uparrow and H_\downarrow correspond to the effective tight-binding Hamiltonians for the up and down spin electrons, respectively. The last term is a constant term which provides a shift in the total energy.

B. Self consistent procedure

With these decoupled Hamiltonians (H_\uparrow and H_\downarrow) of up and down spin electrons, now we start our self consistent procedure considering initial guess values of $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$. For these initial set of values of $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$, we numerically diagonalize the up and down spin Hamiltonians. Then we calculate a new set of values of $\langle n_{i\uparrow} \rangle$ and $\langle n_{i\downarrow} \rangle$. These steps are repeated until a self consistent solution is achieved.

C. The ground state energy

After achieving the self consistent solution, the ground state energy E_0 for a particular filling at absolute zero temperature ($T = 0\text{K}$) can be determined by taking the sum of individual states up to the Fermi energy (E_F) for both the up and down spins. The final expression of the ground state energy is written,

$$E_0 = \sum_n E_{n\uparrow} + \sum_n E_{n\downarrow} - \sum_i U \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \quad (5)$$

where, the index n runs over the states up to the Fermi level. $E_{n\uparrow}$ ($E_{n\downarrow}$) is the single particle energy eigenvalue for n -th eigenstate obtained by diagonalizing the Hamiltonian H_\uparrow (H_\downarrow).

D. Calculation of persistent current

At absolute zero temperature, total persistent current of the system is obtained from the expression [32, 33]

$$I(\phi) = -c \frac{\partial E_0(\phi)}{\partial \phi} \quad (6)$$

where, $E_0(\phi)$ is the ground state energy for a particular filling.

E. Calculation of Drude weight

The conductance can be obtained by calculating the Drude weight D as originally noted by Kohn [39]. The Drude weight for the SPG is obtained through the relation,

$$D = \frac{N}{4\pi^2} \left(\frac{\partial^2 E_0(\phi)}{\partial \phi^2} \right) \Big|_{\phi \rightarrow 0} \quad (7)$$

where, N gives total number of atomic sites in the gasket. Kohn has shown that for an insulating system D decays exponentially to zero, while it becomes finite for a conducting system.

In the present work we inspect all the essential features of magnetic response of an SPG network at absolute zero temperature and use the units where $c = \hbar = e = 1$. Throughout our numerical work we set $\epsilon_{i\uparrow} = \epsilon_{i\downarrow} = 0$ for all i and choose the nearest-neighbor hopping strength $t = -1$. In the anisotropic case we select $t_x = -1$ and $t_y = -2$ throughout. Energy scale is measured in unit of t . Results are obtained both for an isotropic gasket and its anisotropic counterpart.

IV. NUMERICAL RESULTS AND DISCUSSION

In Fig. 2 we present the variation of the ground state energy of a 3-rd generation isotropic SPG containing 15

atomic sites as a function of the magnetic flux through each elementary triangle. Two cases, viz, when the ‘band’ is less than half-filled, and half-filled, are pre-

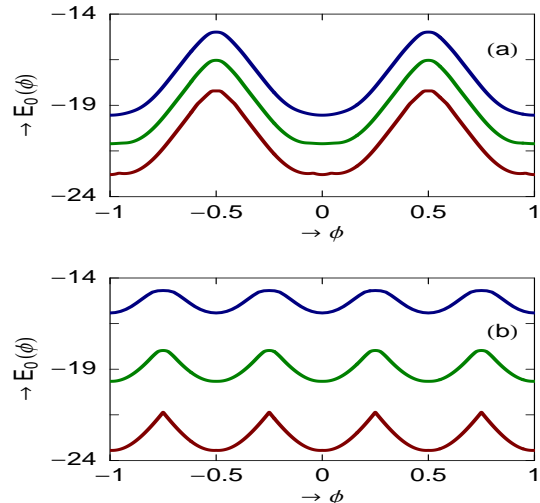


FIG. 2: (Color online). Ground state energy levels as a function of flux ϕ for a 3-rd generation isotropic ($t_x = t_y = -1$) Sierpinski gasket ($N = 15$). The red, green and blue curves correspond to $U = 0, 1$ and 2 , respectively. (a) $N_e = 10$ and (b) $N_e = 15$.

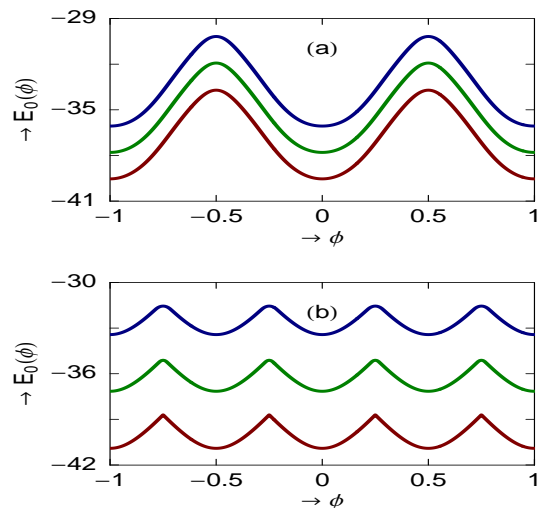


FIG. 3: (Color online). Ground state energy levels as a function of flux ϕ for a 3-rd generation anisotropic ($t_x = -1$ and $t_y = -2$) Sierpinski gasket ($N = 15$). The red, green and blue curves correspond to $U = 0, 1$ and 2 , respectively. (a) $N_e = 10$ and (b) $N_e = 15$.

sented as the on-site Coulomb repulsion U is varied. The ground state energy exhibits a periodicity equal to one flux quantum in all the non-half-filled cases, while the period changes to half flux quantum at precisely half-filling. With increasing U , the ground state energy increases in

both these cases. In the half-filled case, each site is occupied by at least one electron, and the placing of a second electron will increase the energy of the system (the effect of U). This is reflected in Fig. 2(b). Also the values of

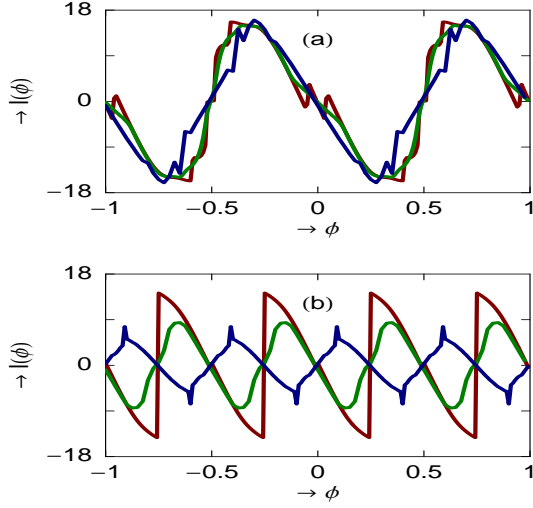


FIG. 4: (Color online). Persistent current as a function of flux ϕ for a 3-rd generation isotropic ($t_x = t_y = -1$) Sierpinski gasket ($N = 15$). The red, green and blue curves correspond to $U = 0, 2$ and 4 , respectively. (a) $N_e = 10$ and (b) $N_e = 15$.

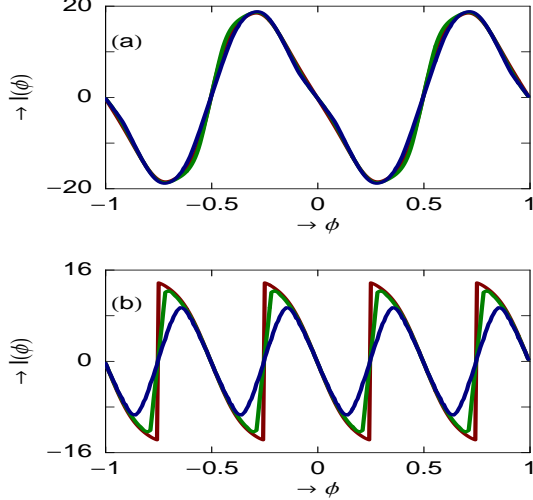


FIG. 5: (Color online). Persistent current as a function of flux ϕ for a 3-rd generation anisotropic ($t_x = -1$ and $t_y = -2$) Sierpinski gasket ($N = 15$). The red, green and blue curves correspond to $U = 0, 2$ and 4 , respectively. (a) $N_e = 10$ and (b) $N_e = 15$.

the ground state energy in the half-filled case turns out to be well separated from each other for $U = 0, 1$ and 2 compared to the non-half-filled case in (a). This feature remains true irrespective of the size of the system.

As anisotropy is introduced, the overall features re-

main unaltered, including the periodicities. However, as is evident from Fig. 3, the anisotropy lowers the ground state energy of an SPG, both in the non-half-filled and the half-filled cases. This will be reflected in the conductance, as will be shown later.

The variation of the persistent current against the magnetic flux is shown separately for the isotropic (Fig. 4) and the anisotropic (Fig. 5) SPG for different values of the Hubbard interaction U . Two typical results, when $N_e = 10$ (less than half-filled case) and $N_e = 15$ (half-filling), are presented for a third generation SPG with $N = 15$ sites. In Fig. 4(a) and in Fig. 5(a) results for the ‘less than half-filled’ case are presented. In Fig. 4(a) the $I(\phi)$ - ϕ curves exhibit multiple kinks which follows from the numerous band-crossings that are typ-

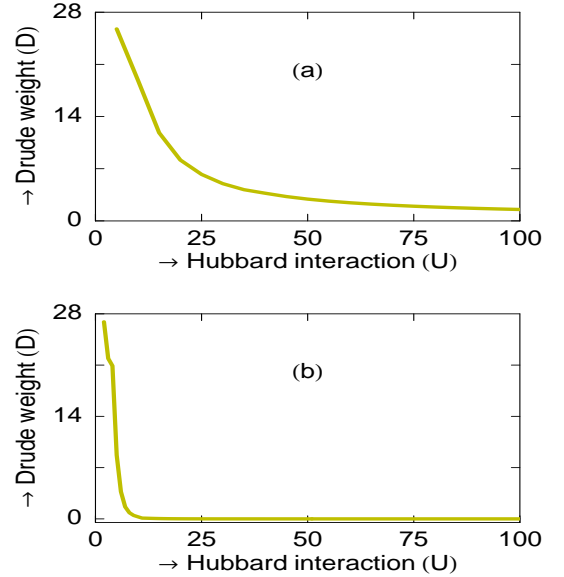


FIG. 6: (Color online). Drude weight as a function of Hubbard interaction strength U for a 3-rd generation isotropic ($t_x = t_y = -1$) Sierpinski gasket ($N = 15$). (a) Non-half-filled case ($N_e = 10$). (b) Half-filled case ($N_e = 15$).

ical of such hierarchical networks [3, 36]. Such crossings become less in number, and global gaps open up in the spectrum, clustering the spectrum into sub-band structures in the case of an anisotropic SPG, as has recently been reported in the literature even in the case of non-interacting electrons [36]. Kinks are now expected to smooth out. That it happens, is evident from the anisotropic case, as depicted in Fig. 5(a). So, anisotropy turns out to be the predominant factor in reducing the band-crossings here.

On the other hand, in the half-filled case, the isotropic version of the SPG display (Fig. 4(b)) non-trivial characteristics compared to its anisotropic counterpart (Fig. 5(b)). In the former case the increasing value of U is seen to result into a complete reversal of the phase of the persistent current, converting a diamagnetic response to a paramagnetic one. This however is not seen

to happen (in the half-filled case) in an anisotropic gasket (Fig. 5(b)).

We now present the results of the calculation of Drude weight D both in the cases of an isotropic and an anisotropic SPG, and observe its variation as U increases. Results are presented in Fig. 6 and Fig. 7, respectively, for a 3-rd generation gasket. It is apparent that, the anisotropic gasket turns out to be more conducting than its isotropic counterpart in the sense that, in the anisotropic case the Drude weight displays finite values over a wider range of U . The magnitude of D at any specific U of course, depends on the numerical values of the hopping strength. Interestingly, this fact is also observed [36] for non-interacting electrons on an SPG. In the half-filled band case, the Drude weight exhibits a much sharper drop in its value compared to the non-half-filled situation. It is true for both the isotropic

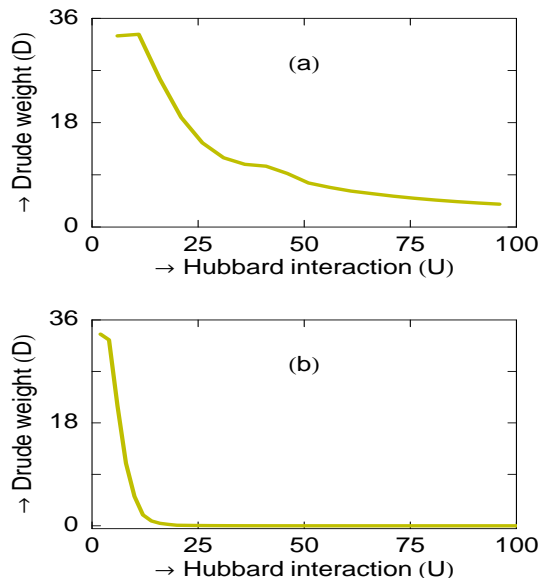


FIG. 7: (Color online). Drude weight as a function of Hubbard interaction strength U for a 3-rd generation anisotropic ($t_x = -1$ and $t_y = -2$) Sierpinski gasket ($N = 15$). (a) Non-half-filled case ($N_e = 10$). (b) Half-filled case ($N_e = 15$).

as well as the anisotropic case. The reason can easily be traced back again to the fact that at half-filling, every site of the SPG network has one electron occupying it already. So, conduction becomes difficult as one needs more energy when an electron tries to leave its own site and occupy a neighboring site. At less than half-filling there are ‘empty’ lattice points and conduction becomes easier. However, we find that in the anisotropic case, we have to make the on-site Hubbard interaction much stronger compared to the isotropic case to lower the value of the conductance close to zero.

Before we end this section, it is pertinent to raise the question as to whether the features discussed above really represent the characteristics of a fractal. To get a definite answer to this, we have extended our analysis to higher

generation SPG networks, both in the isotropic and the anisotropic limits. In each case, the overall features of the ground state energy, the persistent current or the Drude weight turn out to be the same as in the cases of lower generations. The effect of a variation of the Hubbard interaction essentially plays the same role. The difference in the numerical values of the quantities are of course, obvious. To clarify, we provide the results of our calculation on a fourth generation SPG network comprising of 42 sites in the anisotropic limit, and in the half-filled band case. This is in Fig. 8. The ground state energy

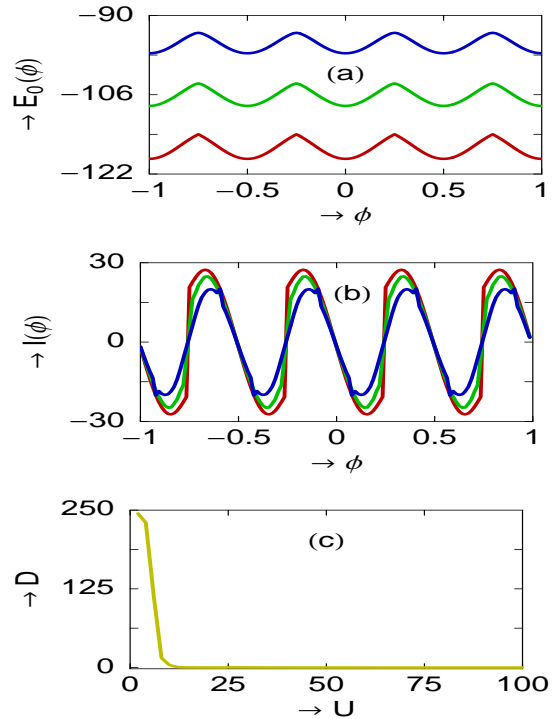


FIG. 8: (Color online). Magnetic response for a 4-th generation anisotropic ($t_x = -1$ and $t_y = -2$) Sierpinski gasket ($N = 42$) in Half-filled case ($N_e = 42$). (a) Energy-flux characteristics where the red, green and blue curves correspond to $U = 0, 1$ and 2 , respectively. (b) Current-flux characteristics where the red, green and blue curves correspond to $U = 0, 2$ and 4 , respectively. (c) Drude weight as a function of Hubbard interaction strength.

in this case, as in the previous generations, exhibits the same qualitative variation against the magnetic flux, and it is the derivative of the ground state energy that generates the current. So, a qualitative similarity between the curves at various generations is not unexpected. A direct comparison with Fig. 5 reveals that, the persistent current for $U = 0$ in the present case is a bit rounded off at the peak compared to the sharp discontinuity exhibited in the corresponding case in the third generation fractal. This is not un-natural, as the current depends on the band crossings exhibited by the eigenvalue spectrum of the finite generation fractals, and the nature of

band crossings will change in every generation. But, the important point to note is that, the periodicity of the persistent current is not affected, and the gradual phase shift shown by the $I(\phi)$ curves in every generation, as the Hubbard interaction is increased, is consistent. The observations remain the same when we go beyond the fourth generation. This attempts us to believe that the features are likely to persist for SPG networks of arbitrarily large finite generations.

V. CLOSING REMARKS

In conclusion, we have performed a thorough mean field analysis of the response of a Sierpinski gasket fractal to an external magnetic field. We have examined both the isotropic and the anisotropic limits of the system, where the anisotropy is introduced only in the values of the nearest-neighbor hopping integrals along two directions. Within the framework of the unrestricted Hartree-Fock theory we decouple the Hubbard Hamiltonian and obtain the ground state energy, the persistent current and

the Drude weight. The persistent current exhibits non trivial patterns in each case, and even reveals a change in response, from diamagnetic to paramagnetic in the isotropic case as a function of the interaction U . So, the Hubbard interaction is seen to play its part in the magnetic response. The band crossing is diminished by the anisotropy. The network remains diamagnetic in the isotropic case, as far as we have examined. The conductance is obtained through the Drude weight and, depending on the values of the nearest-neighbor hopping integrals, the anisotropic gasket may remain conducting than its isotropic counterpart for a wider range of the Hubbard correlation.

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